Physical Chemistry

STRUCTURE OF GOLD CLUSTERS: TWO TO FOURTEEN ATOMS AND TWENTY ATOMS

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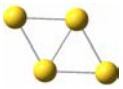
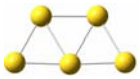
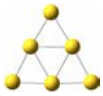
The atomic structures of neutral gold nanoparticle clusters were investigated using the Vienna *ab-initio* Simulation Package (VASP). This package utilizes density functional theory with *ab-initio* pseudopotentials to determine the energy of nanoparticle clusters. The binding energy, E_B, is subsequently calculated using the following equation: $E_B = (E_T - n*E_{atom})/n$, where E_T is the total energy of the cluster, E_{atom} is the energy found in an individual atom, and n is the number of atoms in the cluster.

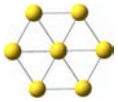
Cluster sizes between two atoms of gold and fourteen atoms of gold were studied, as well as the twenty-atom gold cluster. A planar structure was found to be the most stable in clusters containing up to nine atoms. In a ten-atom cluster, both a stable planar structure and a stable three-dimensional structure was found. The remaining stable structures were three-dimensional. The most stable atomic structures and their binding energies are as follows.

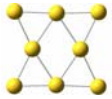
Au_3 1.19 $^{eV}/_{atom}$ 

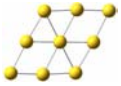
Au_4 1.56 $^{eV}/_{atom}$ 

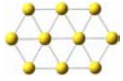
Au_5 1.69 $^{eV}/_{atom}$ 

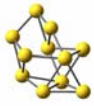
Au_6 1.93 $^{eV}/_{atom}$ 

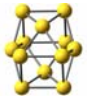
Au_7 1.84 $^{eV}/_{atom}$ 

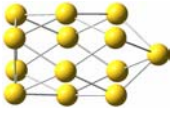
Au_8 2.00 $^{eV}/_{atom}$ 

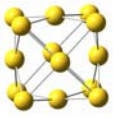
Au_9 1.98 $^{eV}/_{atom}$ 

Au_{10} 2.08 $^{eV}/_{atom}$ 

Au_{11} 2.02 $^{eV}/_{atom}$ 

Au_{12} 2.03 $^{eV}/_{atom}$ 

Au_{13} 2.07 $^{eV}/_{atom}$ 

Au_{14} 2.10 $^{eV}/_{atom}$ 

Au_{20} 2.35 $^{eV}/_{atom}$